Ethanone, 2-amino-1-phenyl-

Other names:	Acetophenone, 2-amino-
	«omega»-Aminoacetophenone
	2-Aminoacetophenone
	Phenacylamine
	2-amino-1-phenylethan-1-one
	2-Amino-1-phenylethanone
Inchi:	InChI=1S/C8H9NO/c9-6-8(10)7-4-2-1-3-5-7/h1-5H,6,9H2
InchiKey:	HEQOJEGTZCTHCF-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	NCC(=O)c1ccccc1
Mol. weight [g/mol]:	135.16
CAS:	613-89-8

Physical Properties

Property code	Value	Unit	Source
gf	66.42	kJ/mol	Joback Method
hf	-50.71	kJ/mol	Joback Method
hfus	17.31	kJ/mol	Joback Method
hvap	53.06	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	0.828		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
ripol	2156.00		NIST Webbook
ripol	2156.00		NIST Webbook
tb	535.52	K	Joback Method
tc	768.22	K	Joback Method
tf	339.53	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.60	J/mol×K	535.52	Joback Method

cpg	255.36	J/mol×K	574.30	Joback Method
cpg	266.29	J/mol×K	613.09	Joback Method
cpg	276.43	J/mol×K	651.87	Joback Method
cpg	285.82	J/mol×K	690.65	Joback Method
cpg	294.50	J/mol×K	729.44	Joback Method
cpg	302.51	J/mol×K	768.22	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C613898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume